Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Monte Carlo simulations of Protein Adsorption SUMIT SHARMA, SANAT K. KUMAR, Columbia University, GEORGES BELFORT, Rensselaer Polytechnic Institute — Amyloidogenic diseases, such as, Alzheimer's are caused by adsorption and aggregation of partially unfolded proteins. Adsorption of proteins is a concern in design of biomedical devices, such as dialysis membranes. Protein adsorption is often accompanied by conformational rearrangements in protein molecules. Such conformational rearrangements are thought to affect many properties of adsorbed protein molecules such as their adhesion strength to the surface, biological activity, and aggregation tendency. It has been experimentally shown that many naturally occurring proteins, upon adsorption to hydrophobic surfaces, undergo a helix to sheet or random coil secondary structural rearrangement. However, to better understand the equilibrium structural complexities of this phenomenon, we have performed Monte Carlo (MC) simulations of adsorption of a four helix bundle, modeled as a lattice protein, and studied the adsorption behavior and equilibrium protein conformations at different temperatures and degrees of surface hydrophobicity. To study the free energy and entropic effects on adsorption, Canonical ensemble MC simulations have been combined with Weighted Histogram Analysis Method(WHAM). Conformational transitions of proteins on surfaces will be discussed as a function of surface hydrophobicity and compared to analogous bulk transitions.

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Date submitted: 13 Dec 2007 Electronic form version 1.4